Herbert Wertheim
College of Engineering
UNIVERSITY *of* FLORIDA

2018 DOE Vehicle Technologies Office
Annual Merit Review Presentation:

Multiscale Development and Validation of the Stainless Steel Alloy Corrosion (SStAC) Tool for High Temperature Engine Materials

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Project ID: mat164

POWERING THE NEW ENGINEER TO TRANSFORM THE FUTURE

Overview

Timeline

- Project start date: Oct 2018
- Project end date: Sept 2021
- Percent complete: 25%

Budget

- Total project funding
  - DOE Share: $1500K
- Funding for FY 2019: $492K
- Funding for FY 2020: $495K

Barriers

- Corrosion of valve materials impact high temperature engines
- Modeling and simulation tools are needed to predict material performance

Partners

- University of Wisconsin-Madison
- Idaho National Laboratory
- TENNECO

Relevance

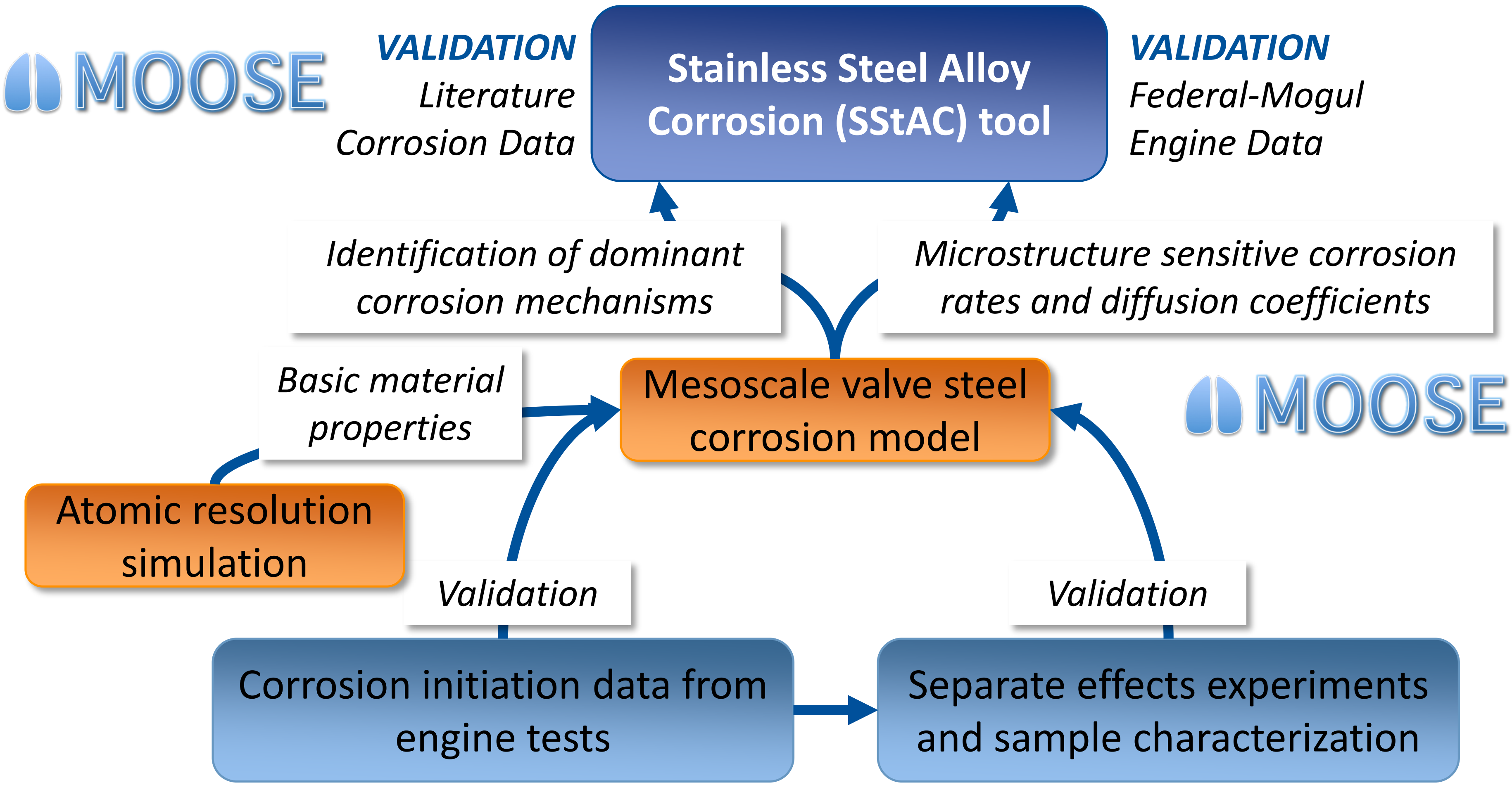
Barrier

- Lack of quantitative understanding of the sensitization of stainless steels to corrosion at high temperature mandates conservative design

Objectives

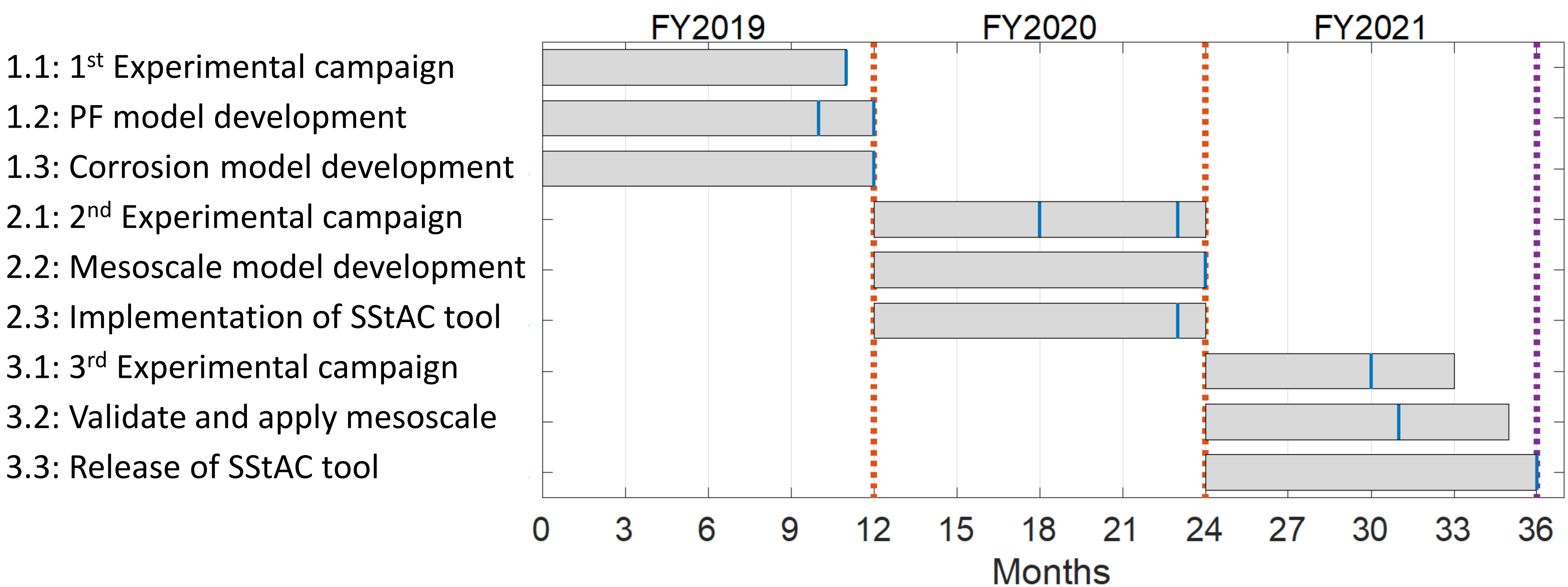
- Develop the open source Stainless Steel Alloy Corrosion (SStAC) tool for modeling corrosion of valve steels in an engine environment.
- Quantify the impact of microstructure and alloy composition on valve steel corrosion using laboratory and engine experiments and mesoscale modeling and simulation.
- Focus is on the 21-2N, 21-4N, and 23-8N valve steel alloys

Approach:
The SStAC tool will be developed using a multiscale approach validated by laboratory and engine data



Approach:
Tasks relating to experiments and modeling will be carried out during all three years of the project

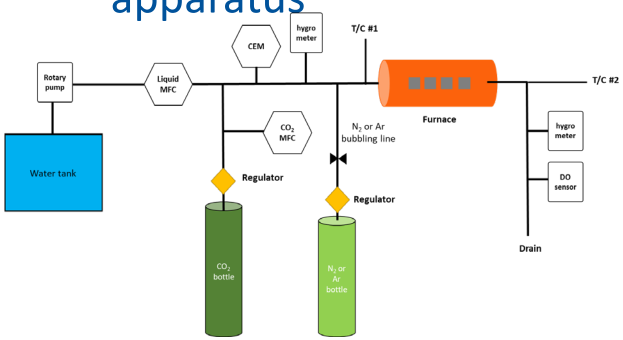
- Tasks 1.1, 2.1, and 3.1 are the three experimental campaigns
- Tasks 1.2, 2.2, and 3.2 are focused on atomic and mesoscale modeling
- Tasks 1.3, 2.3, and 3.3 are focused on the macroscale SStAC tool development



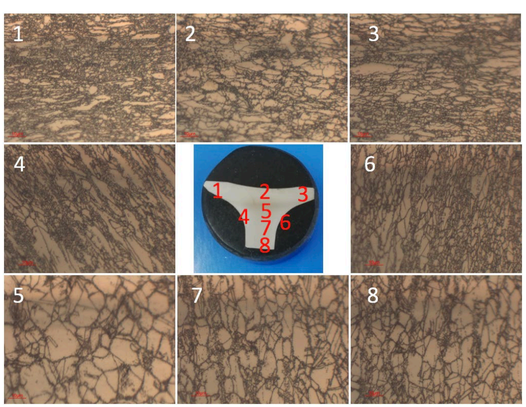
Technical Accomplishments and Progress (6 months):
We have made progress in all three areas of the project

Experiments

- Design of corrosion apparatus

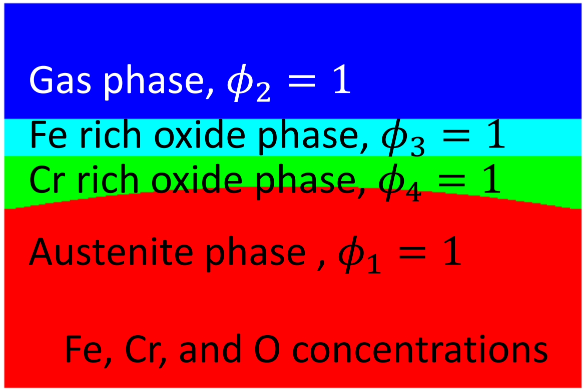


- Characterization of initial valve material



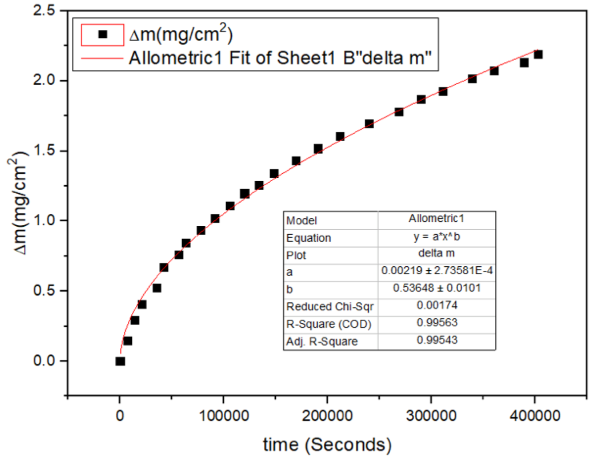
Mesoscale model

- Review of literature of phase field corrosion models
- Formulation of the phase field stainless steel corrosion model



Macroscale model

- Semi-empirical corrosion model is being fit initially to literature data



K_p calculated from

$$\Delta m = a * t^n$$

$$k_p = a = 2.19^{-3} mg.cm^{-2}.S^{-1}$$

With $n = 0.536$

Collaboration and Coordination with Other Institutions

WISCONSIN
UNIVERSITY OF WISCONSIN–MADISON

Developing macroscale SStAC tool, carrying out laboratory corrosion experiments and analyzing corroded samples

INL Idaho National Laboratory

Providing mentorship and guidance on the application and development of the Multiphysics Object-Oriented Simulation Environment

TENNECO

Providing engine valve material, sample preparation, and carrying out engine testing

Proposed Future Research

- Ongoing (FY 2019)
  - Samples of 21-2N and 23-8N valve steel alloys will be corroded at 700 and 800°C
  - Phase field model development. DFT simulations will be used to calculate properties.
  - Macroscale corrosion model development, and model evaluation; Go-No Go
- Future (FY 2020)
  - Corroded samples will be characterized and samples will be corroded with thermal cycling. Engine tests will also be carried out.
  - The phase field model will be coupled with mechanics and electrostatics. DFT simulations will be used to calculate more properties.
  - The SStAC tool will be implemented in MOOSE. The numerical capability of the corrosion tool will be evaluated; Go-No Go

Summary

- The Stainless Steel Alloy Corrosion (SStAC) tool will
  - Be open-source, based on the MOOSE framework
  - Include the impact of microstructure and alloying elements, using information from mesoscale and atomic scale simulations
  - Be validated using new data from laboratory and engine experiments